STRUCTURE SEARCH

```
=> d his 150
    (FILE 'HCAPLUS' ENTERED AT 11:30:06 ON 13 JUL 2009)
           12 S L49 OR L47
L50
               SAV TEMP L50 SAS747HCP/A
=> d que stat 150
L5
                                              G1 16
VAR G1=4/9/14
NODE ATTRIBUTES:
CONNECT IS X2 RC AT 1
CONNECT IS X2 RC AT 3
CONNECT IS E1 RC AT
CONNECT IS E1 RC AT
CONNECT IS X2 RC AT
CONNECT IS E1 RC AT
                      9
CONNECT IS E1 RC AT 10
CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 15
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
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RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 16 STEREO ATTRIBUTES: NONE

C . S . C

1.8

VAR G1=OH/NHZ/ZL/9/11/13/15/17/19/23/26/29

NODE ATTRIBUTES:

HCOUNT IS B1 AT 21

CONNECT IS B1 RC AT 7

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECCOUNT IS M1—X18 C AT 10

ECCOUNT IS M1—X18 C AT 14

ECCOUNT IS M1—X18 C AT 18

GRAPH ATTRIBUTES:

```
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 29
STEREO ATTRIBUTES: NONE
L15
         257255 SEA FILE=REGISTRY SSS FUL L5
L19
                STR
                                                  SAk 021 SE1
                              0--- Ak
09-10
                                         017 CY
 S-CY
            a N- Ak
                       a Nar Sy
                                   Show Source
VAR G1=OH/NH2/21/9/11/13/15/17/19/23/26/29
NODE ATTRIBUTES:
HCOUNT IS E1
CONNECT IS E1 RC AT 7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X18 C AT 10
ECOUNT IS M1-X18 C AT 14
ECOUNT IS M1-X18 C AT 18
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 29
STEREO ATTRIBUTES: NONE
             30 SEA FILE=REGISTRY SUB=L15 SSS FUL L5 AND L19
L22
L24
             18 SEA FILE-REGISTRY SUB-L15 SSS FUL L5 AND L8
L25
                OUE SPE=ON ABB=ON PLU=ON CH2O OR C2H4O OR C3H6O OR
                C4C80
L26
              6 SEA FILE-REGISTRY SPE=ON ABB=ON PLU=ON L24 AND L25
L28
              2 SEA FILE-REGISTRY SPE-ON ABB-ON PLU-ON L24 AND
                75-21-8/CRN
1.30
              O SEA FILE-REGISTRY SPE-ON ABB-ON PLU-ON L24 AND
                75-56-9/CRN
              2 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L22 AND
                75-21-8/CRN
L32
              O SEA FILE-REGISTRY SPE-ON ABB-ON PLU-ON L22 AND
                75-56-9/CRN
          21108 SEA FILE-REGISTRY SPE-ON ABB-ON PLU-ON 553.3/RID
L38
L39
              2 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L24 AND L38
              8 SEA FILE-REGISTRY SPE-ON ABB-ON PLU-ON L26 OR L28
L40
               OR (L30 OR L31 OR L32) OR L39
L43
             30 SEA FILE-REGISTRY SPE-ON ABB-ON PLU-ON L22 OR L24
L44
                QUE SPE=ON ABB=ON PLU=ON PY=<2003 NOT P/DT
L45
                QUE SPE=ON ABB=ON PLU=ON (PY=<2003 OR PRY=<2003 OR
               AY=<2003 OR MY=<2003 OR REVIEW/DT) AND P/DT
T.46
             17 SEA FILE-HCAPLUS SPE-ON ABB-ON PLU-ON L43
L47
             12 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L46 AND (L44
               OR L45)
L48
              3 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L40
L49
            1 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L48 AND L47
12 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L49 OR L47
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L50

STRUCTURE SEARCH RESULTS

=> d 150 1-12 ibib ed abs hitstr hitind

L50 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2005:568976 HCAPLUS Full-text

DOCUMENT NUMBER: 143:83603 TITLE: One-part self-etchi

TITLE: One-part self-etching, self-priming dental

adhesive composition

INVENTOR(S): Klee, Joachim E.; Lehmann, Uwe; Walz, Uwe

PATENT ASSIGNEE(S): Dentsply Detrey GmbH, Germany SOURCE: Eur. Pat. Appl.. 30 pp.

SOURCE: Eur. Pat. Appl., 30 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Fatent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PR

| TENT | INFOR | MATI | ON: | | | | | | | | | | | | |
|--------|---------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|----------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|-------------------|--------------------------|
| | | | | | | KIND | | DATE | | APPLICATION NO. | | | | DATE | |
| | 1548 | | | | A1 | | 2005 | 0629 | | EP 2 | 003- | 2982 | 4 | | 2003 |
| EP | 1548 R: | AT, | | | DE, | DK | 2007 ES, | FR, | GB, | GR, | | | | | |
| AT | 3574 | EE, | HU, | | | | , LV, 2007 | | | | | | | во, | 2003 |
| CA | 2551 | 228 | | | A1 | | 2005 | 0714 | | | 004- | 2551: | 228 | | 2004 |
| Wo | 2005 | 0637 | 78 | | A1 | | 2005 | 0714 | , | | 004- | EP14 | 307 | | 1215 2004 |
| | w. | ΔF | 16 | 21. | ΔM | ΔT | , AU, | 2.7 | R2 | | BG | RP. | RW | RV | 1215 |
| | ". | CA, ES, KE, MG, PT, | CH, FI, KG, MK, RO, | CN, GB, KP, MN, RU, | CO, GD, KR, MW, SC, | CR GE KZ MX SD | CU, GH, LC, MZ, SE, | CZ, GM, LK, NA, SG, | DE, HR, LR, NI, SK, | DK, HU, LS, NO, SL, | DM, ID, LT, NZ, SY, | DZ, IL, LU, OM, TJ, | EC, IN, LV, PG, TM, | EE, IS, MA, | EG, JP, MD, PL, |
| | RW: | BW, ZW, CY, LT, | GH, AM, CZ, LU, | GM, AZ, DE, MC, | KE, BY, DK, NL, | LS KG EE PL | MW, KZ, ES, PT, | MZ, MD, FI, RO, | NA, RU, FR, SE, | SD, TJ, GB, SI, | SL, TM, GR, SK, | SZ, AT, HU, TR, | TZ, BE, IE, BF, | IS, BJ, | CH, IT, |
| JP | 2007 | 5204 | 65 | | T | | 2007 | 0726 | | | 006- | 5459 | 98 | | 2004 1215 |
| US | 20 0 7 | 0293 | 642 | | A1 | | 2007 | 1220 | | US 2 | 007- | 5967 | 47 | | 2007 0508 |
| RIORIT | Y APP | LN. | INFO | .: | | | | | | | 003- | 2982 | 4 | i | A 2003 1223 |
| | | | | | | | | | | < | | | | | |

Page 3

WO 2004-EP14307 W

2004 1215

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Entered STN: 01 Jul 2005
AB
     One-part self-etching, self-priming dental adhesive composition having a pH of at most
     2 comprises (a) a polymerizable acidic phosphoric acid ester monomer; (b) one or more
     polymerizable acidic monomers; (c) a polymerizable N-substituted alkylacrylic or
     acrylic acid amide monomer; (d) an organic and/or inorg. acid; (e) an organic water
     soluble solvent and/or water; and (f) polymerization initiator, inhibitor and
     stabilizer. An adhesive polymer was prepared from 2-acrylamido-2-methyl-propane-
     sulfonic acid, 3, (4), 8, (9)-bis(acrylamido methyl) tricyclo-5.2.1.02,6 decane, Et 2-[13-
     dihydrogen phosphoryl-13,2-dioxatridecyl]acrylate, and N,N'-bisacrylamido-N,N'-diethyl-
     1,3-propane.
    752234-98-3P 752235-00-0P 855894-56-3P
TT
     RL: IMF (Industrial manufacture); RCT (Reactant); PREP
     (Preparation); RACT (Reactant or reagent)
        (one-part self-etching, self-priming dental adhesive composition)
     752234-98-3 HCAPLUS
CN
     2-Propenoic acid, 2-[[[10-(phosphonooxy)decyl]oxy]methyl]-,
     1-ethyl ester (CA INDEX NAME)
 Eto____CH2__o_ (CH2)10__OPO3H2
RN
     752235-00-0 HCAPLUS
     2-Propenoic acid, 2-[[2-(phosphonooxy)ethoxy]methyl]-, 1-ethyl
CN
     ester (CA INDEX NAME)
 Eto_U_U_GH2_O_GH2_GH2_OPO3H2
     855894-56-3 HCAPLUS
RN
CM
     2-Propenoic acid, 2-[[2-(phosphonooxy)ethoxy]methyl]- (CA INDEX
    NAME)
 HO . C. . CH . _ O_ CH . _ CH . _ OPO 3H .
   855894-57-4F, 2-Acrylamido-2-methyl-propane-sulfonic
     acid-3,(4),8,(9)-bis(acrylamido methyl) tricyclo-5.2.1.02,6
     decane-Ethvl 2-[13-dihydrogen
     phosphoryl-13, 2-dioxatridecyl acrylate-N, N'-Bisacrylamido-N, N'-
     diethyl-1,3-propane copolymer 855894-58-59
     RL: IMF (Industrial manufacture); THU (Therapeutic use); BIOL
     (Biological study); PREP (Preparation); USES (Uses)
        (one-part self-etching, self-priming dental adhesive composition)
RN
    855894-57-4 HCAPLUS
     2-Propenoic acid, 2-[[[10-(phosphonooxy)decyl]oxy]methyl]-,
     1-ethyl ester, polymer with
     2-methyl-2-[(1-oxo-2-propen-1-yl)amino]-1-propanesulfonic acid,
     N.N-[[octahydro-4,7-methano-1H-indene-1,5(1,6 or
     2,5)diyl|bis(methylene)|bis[2-propenamide] and
     N, N'-1, 3-propanediylbis[N-ethyl-2-propenamide] (CA INDEX NAME)
```

RN 855894-58-5 HCAPLUS

CN 2-Propenoic acid, 2-[[2-(phosphonooxy)ethoxy]methyl]-, 1-ethyl ester, polymer with 2-methyl-2-[(1-oxo-2-propenyl)amino]-1-

propanesulfonic acid, N,N-[[octahydro-4,7-methano-1H-indene-1,5(1,6 or 2,5)diyl]bis(methylene)]bis[2-propenamide] and N,N'-1,3-propanediylbis[N-ethyl-2-propenamide] (9CI) (CA INDEX NAME)

CM 1

CRN 855532-00-2 CMF C18 H26 N2 O2

CCI IDS

CM 2

CRN 752235-00-0 CMF C8 H15 O7 P

CM 3

CRN 442200-41-1 CMF C13 H22 N2 O2

CM

CRN 15214-89-8 CMF C7 H13 N O4 S

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IC ICM C07F009-09
    ICS C08F030-02; A61K006-00; A61K006-083
    63-8 (Pharmaceuticals)
    752234-97-2P 752234-98-3P 752234-99-4P
    752235-00-0P 855894-56-3P
     RL: IMF (Industrial manufacture); RCT (Reactant); PREP
     (Preparation); RACT (Reactant or reagent)
       (one-part self-etching, self-priming dental adhesive composition)
IT 855834-57-4P, 2-Acrylamido-2-methyl-propane-sulfonic
     acid-3,(4),8,(9)-bis(acrylamido methyl) tricyclo-5.2.1.02,6
    decane-Ethyl 2-[13-dihydrogen
     phosphoryl-13, 2-dioxatridecyl]acrylate-N, N'-Bisacrylamido-N, N'-
     diethyl-1,3-propane copolymer 855894~58~5P
     RL: IMF (Industrial manufacture); THU (Therapeutic use); BIOL
     (Biological study); PREP (Preparation); USES (Uses)
       (one-part self-etching, self-priming dental adhesive composition)
REFERENCE COUNT:
                      5
                             THERE ARE 5 CITED REFERENCES AVAILABLE
                             FOR THIS RECORD. ALL CITATIONS AVAILABLE
                             IN THE RE FORMAT
L50 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:182218 HCAPLUS Full-text
DOCUMENT NUMBER:
                       142:287808
TITLE:
                      Lithographic printing plate precursor for
                       direct imaging from a digital data and
                       developing in a printing machine without
                      passing through a development step
INVENTOR(S):
                       Yamasaki, Sumiaki; Makino, Naonori; Inno,
                       Toshifumi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE:
                       U.S. Pat. Appl. Publ., 50 pp.
                       CODEN: USXXCO
DOCUMENT TYPE:
                      Patent
LANGUAGE .
                       English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
     PATENT NO. KIND DATE APPLICATION NO.
    PATENT NO.
    US 20050048398
                      Al 20050303 US 2004-896070
                                                                2004
                                                                0722
                                            <--
    US 7183038 B2 20070227
EP 1500498 A2 20050126
                                       EP 2004-17306
                                                                2004
                                                                0722
                                            <--
    EP 1500498
                       A3 20051012
        R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR,
            HU, IE, IT, LI, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR
     JP 2005238816
                       A
                            20050908 JP 2004-214190
                                                                2004
                                                               0722
                                            <--
                                          JP 2003-277448
PRIORITY APPLN. INFO .:
                                                                2003
                                                                0722
                                          JP 2004-652
                                                                2004
                                                                0105
                                          JP 2004-17599 A
```

2004 0126 JP 2004-214190 A 2004 0722

OTHER SOURCE(S): MARPAT 142:287808

ED Entered STN: 04 Mar 2005

- AB A lithog, printing plate precursor is described for recording an image directly from a digital data and development in a printing machine without passing through a development step. The precursor provides lithog, printing plates with improved press life and stain resistance. Thus, the precursor coating composition comprises an image-forming layer containing a polymerization initiator and a polymerizable compound, and a hydrophilic support. The composition includes a compound containing at least one functional group interacting with a surface of the hydrophilic support. This compound is one of a phosphonic acid and a phosphoric acid amide.
 - T 847226-71-5

RL: TEM (Technical or engineered material use); USES (Uses) (lithog, printing plate precursor for direct imaging from digital data and in-press development)

RN 847226-71-5 HCAPLUS

CN 2-Propenoic acid, 2-(15,15-dihydroxy-15-oxido-2,5,8,11,14-pentaoxa-15-phosphapentadec-1-y1)-, 1-ethyl ester (CA INDEX NAME)

PAGE 1-B

- OPO3H2

IT 847204-83-5 847204-84-6

RL: TEM (Technical or engineered material use); USES (Uses) (phosphonic derivative; lithog. printing plate precursor for direct imaging from digital data and in-press development)

RN 847204-83-5 HCAPLUS

CN 2-Propenoic acid, 2-(9,9-dihydroxy-9-oxido-2,5,8-trioxa-9-phosphanon-1-y1)-, 1-methyl ester (CA INDEX NAME)

O CH2 MeO_U_U_CH2_O_CH2_CH2_O_CH2_CH2_OPO3H2

RN 847204-84-6 HCAPLUS

CN 2-Propenoic acid, 2-(15,15-dihydroxy-15-oxido-2,5,8,11,14-pentaoxa-15-phosphapentadec-1-yl)-, 1-methyl ester (CA INDEX NAME)

PAGE 1-A

O CH2
(eQ_U_U_CH2_O_CH2_CH2_CH2_O_CH2_OH2_OH2_OH2_CH2_O

PAGE 1-B

- OP03H2

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IC ICM 603C001-492
INCL 430270100
C 74-5 (Rediation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
I 847204-89-9 847204-89-0 847204-89-1 847204-90-4
847204-91-5 847226-71-5
RE: TBM (Technical or engineered material use); USES (Uses)
(11thog. printing plate precursor for direct imaging from digital data and in-press development)
```

IT 80730-17-2 223681-84-3 847204-73-3 847204-74-4 847204-75-5 847204-76-6 847204-77-7 847204-78-8 847204-82-4 847204-89-5 847204-84-6 847204-85-7

847232-64-8

RL: TEM (Technical or engineered material use); USES (Uses)

(phosphonic derivative; lithog. printing plate precursor for direct imaging from digital data and in-press development)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE

FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2009 ACS ON STN ACCESSION NUMBER: 2004:732258 HCAPLUS Full-text DOCUMENT NUMBER: 141:243056

TITLE: Polymerizable phosphoric acid ester

derivatives for dental compositions
INVENTOR(S): Klee, Joachim E.; Lehmann, Uwe; Walz, Uwe;

Liu, Huaibing
PATENT ASSIGNEE(S): Dentsply Detrey GmbH, Germany

SOURCE: Eur. Pat. Appl., 20 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

> PATENT NO. KIND DATE APPLICATION NO. DATE EP 1454911 A1 20040908 EP 2003-5174 2003 0307 /__ R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK CA 2518202 A1 20040916 CA 2004-2518202 2004 0305 WO 2004078100 A2 20040916 WO 2004-EP2289 2004

W0 2004078100 A3 20041028
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ,

0305

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CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG,
             ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
             KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,
            MG, MK, MN, MW, MX, MZ, NA, NI
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW,
            AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR,
            HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF,
            BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1601679
                         A.2
                             20051207 EP 2004-717576
                                                                   2004
                                                                   0305
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,
            MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ,
            EE, HU, PL, SK
     JP 2006520344
                                20060907
                                           JP 2006-504563
                                                                   2004
                                                                   0305
    US 20060246017
                       Al
                               20061102
                                            US 2006-548362
                                                                   2006
                                                                   0626
PRIORITY APPLN. INFO.:
                                            EP 2003-5174
                                                                   2003
                                                                   0307
                                               <--
                                            WO 2004-EP2289
                                                                   2004
                                                                   0305
```

- ED Entered STN: 09 Sep 2004
- AB The present invention provides a polymerizable phosphoric acid ester derivative for use in dental compns. E.g., 2, 2, 2-tris(2,6-drioxa-4-methylene-5-oxo-octyl)ethanol phosphoric acid ester was prepared from pentaerythritol, Et chloromethyacrylate, and then treatment with the product with POCI3 and hydrolyzed.
- IT 752234-96-1P 752234-98-3P 752235-00-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (polymerizable phosphoric acid ester derivs. for dental

- compns.)
- RN 752234-96-1 HCAPLUS
 CN 2-Propenoic acid, 2,2'-[[2-[[[2-(ethoxycarbonyl)-2-

propenyl]oxy]methyl]-2-[(phosphonooxy)methyl]-1,3propanediyl]bis(oxymethylene)]bis-, 1,1'-diethyl ester (9CI) (CA INDEX NAME)

- RN 752234-98-3 HCAPLUS
- CN 2-Propenoic acid, 2-[[[10-(phosphonooxy)decyl]oxy]methyl]-, 1-ethyl ester (CA INDEX NAME)

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752235-00-0 HCAPLUS
     2-Propenoic acid, 2-[[2-(phosphonooxy)ethoxy]methyl]-, 1-ethyl
     ester (CA INDEX NAME)
 Eto_U_CH2_O_CH2_CH2_OPO3H2
TC
     ICM C07F009-09
     ICS A61K006-08; C08F030-02
     23-17 (Aliphatic Compounds)
     Section cross-reference(s): 63
     752234-96-1P 752234-98-3P 752235-00-0P
     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL
     (Biological study); PREP (Preparation); USES (Uses)
        (polymerizable phosphoric acid ester derivs. for dental
        compns.)
REFERENCE COUNT:
                               THERE ARE 4 CITED REFERENCES AVAILABLE
                               FOR THIS RECORD. ALL CITATIONS AVAILABLE
                               IN THE RE FORMAT
L50 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:
                         2003:69754 HCAPLUS Full-text
DOCUMENT NUMBER:
                         139:65615
TITLE:
                         A fluorescent sensor for
                         2,3-bisphosphoglycerate using a europium
                         tetra-N-oxide bis-bipyridine complex for both
                         binding and signaling purposes
AUTHOR(S):
                         Best, Michael D.; Anslyn, Eric V.
CORPORATE SOURCE:
                         The University of Texas at Austin, Austin, TX,
                         78712-1167, USA
SOURCE:
                         Chemistry--A European Journal (2003
                         ), 9(1), 51-57
                         CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER:
                         Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
ED
     Entered STN: 29 Jan 2003
     Host 1 was designed and synthesized as a fluorescent sensor for 2,3-bisphosphoglycerate
     (BPG, 3). The design features a tris-functionalized triethylbenzene core to
     preorganize binding groups. The three cationic moieties, a tetra-N-oxide bipyridine-
     europium complex and two ammonium groups, were included to complement the three anionic
     functionalities on the quest. Beyond acting as a binding site, the europium complex was
     used to signal binding of the quest through modification of the charge transfer
     emission. A 1:1 complex with BPG was determined in 50% methanol/acctonitrile with a Ka
     of 6.7+105 mol-1 by monitoring the reduction of the fluorescence signal upon guest
     addition In the titration of related glycolytic intermediates lacking a second
     phosphate (4-6) into host 1, 2:1 host to guest binding was observed Similarly, control
     compound 2, which lacks the ammonium groups, binds BPG and 4-6 in a 2:1 fashion. Also,
     phenylphosphate 7 binds to host 1 in a 1:1 stoichiometry with a Ka over three times
     less than 3.
TT
     549507-60-0
     RL: ARU (Analytical role, unclassified); ANST (Analytical study)
        (fluorescent sensor for 2,3-bisphosphoglycerate using europium
        tetra-N-oxide bis-bipyridine complex for both binding and
        signaling purposes)
    549507-60-0 HCAPLUS
     2-Propenoic acid, 2-[(phosphonooxy)methyl]- (CA INDEX NAME)
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HO2C_U_CH2_OPO3H2
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9-5 (Biochemical Methods)
    138-81-8 701-64-4 820-11-1 2553-59-5 549507-60-0
     RL: ARU (Analytical role, unclassified); ANST (Analytical study)
        (fluorescent sensor for 2,3-bisphosphoglycerate using europium
        tetra-N-oxide bis-bipyridine complex for both binding and
        signaling purposes)
REFERENCE COUNT:
                         59
                               THERE ARE 59 CITED REFERENCES AVAILABLE
                               FOR THIS RECORD. ALL CITATIONS AVAILABLE
                               IN THE RE FORMAT
L50 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:
                        1997:118009 HCAPLUS Full-text
DOCUMENT NUMBER:
                         126:222078
ORIGINAL REFERENCE NO.: 126:42871a,42874a
TITLE:
                        Purification and preliminary characterization
                         (E)-3-(2,4-dioxo-6-methyl-5-pyrimidinyl)acryli
                         c acid synthase, and enzyme involved in
                         biosynthesis of the antitumor agent
                         sparsomycin
AUTHOR(S):
                         Parry, Ronald J.: Hovt, Jeffrey C.
CORPORATE SOURCE:
                         Dep. of Chemistry, Rice University, Houston,
                         TX, 77251, USA
                         Journal of Bacteriology (1997),
SOURCE .
                         179(4), 1385-1392
                         CODEN: JOBAAY: ISSN: 0021-9193
PUBLISHER:
                         American Society for Microbiology
DOCUMENT TYPE:
LANGUAGE:
                         English
     Entered STN: 20 Feb 1997
ED
AB
     Sparsomycin is an antitumor antibiotic produced by Streptomyces sparsogenes.
     Biosynthetic expts. have previously demonstrated that one component of sparsomycin is
     derived from L-tryptophan via the intermediacy of (E)-3-(4-oxo-6-methyl-5-
     pyrimidinyl)acrylic acid and (E)-3-(2,4-dioxo-6-methyl-5-pyrimidinyl)acrylic acid. An
     enzyme which catalyzes the conversion of (E)-3-(4-oxo-6-methyl-5-pyrimidinyl)acrylic
     acid to (E)-3-(2.4-dioxo-6-methyl-5-pyrimidinyl)acrylic acid was purified 740-fold to
     homogeneity from S. sparsogenes. The mol. mass of the native and denatured enzyme was
     87 kDa, indicating that the native enzyme is monomeric. The enzyme required NAD for
     activity but lacked rigid substrate specificity, since analogs of both inhibited by
     mycophenolic acid. Monovalent cations were required for activity, with potassium ions
     being the most effective. The enzyme exhibited sensitivity toward diethylpyrocarbonate
     and some thiol-directed reagents, and it was irreversibly inhibited by 6-chloropurine.
     The properties of the enzyme suggest it is mechanistically related to inosine-5'-
     monophosphate dehydrogenase.
     73435-45-7, NADX
     RL: BPR (Biological process); BSU (Biological study,
     unclassified); BIOL (Biological study); PROC (Process)
        (substrate; purification and preliminary characterization of
        (E)-3-(2,4-dioxo-6-methyl-5-pyrimidinyl)acrylic acid synthase,
        and enzyme involved in biosynthesis of the antitumor agent
        sparsomycin)
     73435-45-7 HCAPLUS
RN
     Adenosine 5'-(trihydrogen diphosphate), P'→5'-ester with
     2-formy1-3-(β-D-ribofuranosylamino)-2-propenamide (9CI) (CA
     INDEX NAME)
```

Absolute stereochemistry. Double bond geometry unknown.

PAGE 1-B

__ NH 2

7-2 (Enzymes)

53-84-9, B-NAD 68-94-0, Hypoxanthine 4562-27-0, 4-Hvdroxvpvrimidine 7298-93-3, α-NAD 28277-67-0, Uracil acrylic acid 73435-45-7, NADX RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (substrate; purification and preliminary characterization of (E)-3-(2.4-dioxo-6-methyl-5-pyrimidinyl)acrylic acid synthase.

and enzyme involved in biosynthesis of the antitumor agent sparsomycin) REFERENCE COUNT: THERE ARE 36 CITED REFERENCES AVAILABLE 36 FOR THIS RECORD. ALL CITATIONS AVAILABLE

IN THE RE FORMAT L50 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:684772 HCAPLUS Full-text DOCUMENT NUMBER: 125:303429

ORIGINAL REFERENCE NO.: 125:56755a,56758a

TITLE: Phosphoric acid esters and their manufacture, and polymers from them

INVENTOR(S):

Nagano, Hideaki; Yurugi, Keiji; Nakagawa, Koichi: Kita, Juichi

Nippon Catalytic Chem Ind. Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT ASSIGNEE(S):

| PATENT INFORMATION: | | | | | |
|------------------------|------|----------|--------------------|--------------|--|
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE | |
| JP 08231564 | A | 19960910 | JP 1995-40604 | 1995 0228 | |
| PRIORITY APPLN. INFO.: | | | < JP 1995-40604 | 1995 | |
| | | | | 0228 | |

OTHER SOURCE(S): MARPAT 125:303429

ED Entered STN: 20 Nov 1996

Polymers [number-average mol. weight (Mn) 1000-1,000,000] having units AB CH2CXCHR1OP(0)(OH)2 and/or CH2CXCHR1OP(0)(OH)OCHR1CXCH2, useful for coatings with

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10/596.747-301496-EIC SEARCH
     excellent adhesion, etc., are obtained from [CH2:CXCHR10]nP(0)(OH)3-n, which are
     manufactured from P compds. and CH2:CXCHR10H (R1 = H, organic residues; X = CN, COR2,
     CO2R2; R2 = organic residues; n = 1-2). Thus, 39 g Et \alpha-hydroxymethyl acrylate was
     treated with 21.3 g P205 at 50° for 4 h in the presence of hydroguinone monomethyl
     ether, hydrolyzed, and polymerized at 80° in the presence of 2,2'-
     azobisisobutylonitrile to give a polymer (Mn 45,000). Then, 25 g polymer was blended with 25 g 1,6-hexanediol diacrylate, 3 g Irgacure 651, and 50 g urethane acrylate
     manufactured from isophorone diisocvanate 2, triethylene glycol 1, and 2-hydroxyethyl
     acrylate 2 mols, applied on a steel plate, and cured by irradiation of UV to show
     cross-cut adhesion 100/100.
   183175-03-3P 183175-04-4P
     RL: IMF (Industrial manufacture): MOA (Modifier or additive use);
     TEM (Technical or engineered material use); PREP (Preparation);
     USES (Uses)
        (manufacture of allyl alc. phosphoric acid ester polymers for
       coatings with good adhesion)
RM
    183175-03-3 HCAPLUS
CN
    Propanedioic acid, methylene-, ethyl 2-(phosphonooxy)ethyl ester,
    homopolymer (9CI) (CA INDEX NAME)
    CRN 183175-01-1
    CMF C8 H13 O8 P
 Eto_U_C_0_CH2_CH2_OP03H2
    183175-04-4 HCAPLUS
CM
     4,7,9,12-Tetraoxa-8-phosphapentadecanedioic acid,
     8-hydroxy-2,14-bis(methylene)-3,13-dioxo-, diethyl ester, 8-oxide,
     polymer with ethenylbenzene (9CI) (CA INDEX NAME)
    CM 1
    CRN 183175-02-2
    CMF C16 H23 O12 P
```

H2C___CH_Ph

CM 2 CRN 100-42-5 CMF C8 H8

T 183175-01-19 183175-02-2P RL: IMF (Industrial manufacture); RCT (Reactant); PREP

(Preparation); RACT (Reactant or reagent) (manufacture of allyl alc. phosphoric acid ester polymers for coatings with good adhesion)

RN 183175-01-1 HCAPLUS

CN Propanedioic acid, 2-methylene-, 1-ethyl 3-[2-(phosphonooxy)ethyl] ester (CA INDEX NAME)

$$\texttt{Eto} = (\begin{matrix} \texttt{CH2} \\ \texttt{L} \\ \texttt{L} \end{matrix} , \begin{matrix} \texttt{CH2} \\ \texttt{L} \end{matrix} , \begin{matrix} \texttt{CH2} \\ \texttt{CH2} \end{matrix})$$

RM 183175-02-2 HCAPLUS

CN 4,7,9,12-Tetraoxa-8-phosphapentadecanedioic acid, 8-hydroxy-2,14-bis(methylene)-3,13-dioxo-, diethyl ester, 8-oxide (9CI) (CA INDEX NAME)

$$\texttt{Eto} = \bigcup_{k=0}^{k-1} \bigcup_{k=0}^{k-2} \bigcup_{k=$$

IC ICM C07F009-09 TCS C08F030=02

ICA C09D007-12

42-10 (Coatings, Inks, and Related Products) Section cross-reference(s): 23, 35

183175-03-3P 183175-04-4P

RL: IMF (Industrial manufacture); MOA (Modifier or additive use); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(manufacture of allyl alc. phosphoric acid ester polymers for coatings with good adhesion)

183175-01-1P 183175-02-2P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(manufacture of allyl alc. phosphoric acid ester polymers for

coatings with good adhesion) L50 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1996:368751 HCAPLUS Full-text

DOCUMENT NUMBER: 125:168619

ORIGINAL REFERENCE NO.: 125:31613a,31616a TITLE: Novel phosphotyrosine mimetics in the design

of peptide ligands for pp60src SH2 domain AUTHOR(S): Shahripour, Aurash; Plummer, Mark S.; Lunney, Elizabeth; Para, Kimberly S.; Stankovic,

Charles J.; Rubin, John R.; Humblet,

Christine: Fergus, James H.; Marks, James S.; et al.

CORPORATE SOURCE: Dep. Chem., Parke-Davis Pharm. Res., Ann

Arbor, MI, 48105, USA SOURCE . Bioorganic & Medicinal Chemistry Letters (

1996), 6(11), 1209-1214 CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier DOCUMENT TYPE: Journal LANGUAGE: English

ED Entered STN: 26 Jun 1996

AB The authors have designed and synthesized a series of phosphorylated penta- and tripeptides of general structures R-Glu-Glu-Ile-Glu-OH and R-Glu-D-Trp-HH2, where R represents a phosphotyrosine mimetic. These peptides show binding affinity to pp50src SH2 domain in the micromolar range. Data are presented that provide an account of their structure-activity relationships and specificity properties.

179984-94-29

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BTOL (Biological study); PREP (Preparation)

(prepn of novel phosphotyrosine mimetics in the design of peptide ligands for pp60src SH2 domain)

RN 179984-94-2 HCAPLUS

CN L-Glutamic acid, N-[N-[N-[N-[2-carboxy-1-oxo-3-[4-

(phosphonooxy)phenyl]-2-propenyl]-L- α -glutamyl]-L- α -glutamyl]-L-isoleucyl]-, (Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

CC 34-3 (Amino Acids, Peptides, and Proteins) Section cross-reference(s): 1, 7

179984-85-1P 179984-86-2P ΙT 159439-02-8P 179984-84-0P 179984-87-3P 179984-88-4P 179984-89-5P 179984-90-8P 179984-91-9P 179984-92-0P 179984-93-1P 179984-94-2P 179985-01-4P 179984-96-4P 179984-99-7P 179985-03-6P 179985-05-8P 179985-06-9P 179985-08-1P 179985-09-2P 179985-11-6P 180184-68-3P 180184-69-4P 180184-70-7P 180184-71-8P 180184-72-9P 180184-73-0P 180184-74-1P 180184-75-2P 180184-76-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn of novel phosphotyrosine mimetics in the design of peptide ligands for pp60src SH2 domain)

L50 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1995:603791 HCAPLUS Full-text

DOCUMENT NUMBER: 123:17973

ORIGINAL REFERENCE NO.: 123:3351a,3354a

TITLE: surface coating of contact lenses

INVENTOR(S): Inomata, Kyoshi; Nakada, Shinji; Koinuma,

Yasuyoshi; Nakabayashi, Norio; Ishihara, Kazuhiko

PATENT ASSIGNEE(S): Nippon Oils & Fats Co Ltd, Japan; Nakabayashi

Norio

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|---------------------|--------------|
| JP 07072430 | A | 19950317 | JP 1993-218890 | 1993 0902 |
| PRIORITY APPLN. INFO.: | | | < JP 1993-218890 | 1993 0902 |

- ED Entered STN: 10 Jun 1995
- AB The surface of contact leses is coated with phospholipid-like vinyl monomers by graftcopolymn. to give surface-coated contact lenses having hydrophilicity, good wettability, and stain-resistance. Thus, y
 - methacryloyloxypropyltris(trimethyloxy)slane, 2,2,2-trifluoroethyl methacrylate, Me methacrylate and ethylene glycol dimethacrylate were reacted and made into contact lenses, which were graft-copolymd. with
 - 2-(methacroloyloxy)ethyl-2'-(trimethylammonio)ethylphosphate and triethylene glycol dimethacrylate for surface coating.
- IT 163674-38-2P

RL: DEV (Device component use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

- (surface coating of contact lenses)
- RN 163674-38-2 HCAPLUS
 - 2,5,8,10-Tetraoxa-9-phosphadodecan-12-aminium,
 - 3-(1-carboxyethenyl)-9-hydroxy-N,N,N-trimethyl-4-oxo-, inner salt,
 - 9-oxide, polymer with 1,2-ethanediyl bis(2-methyl-2-propenoate), 1,2-ethanediylbis(oxy-2,1-ethanediyl) bis(2-methyl-2-propenoate),
 - methyl 2-methyl-2-propenoate, 2,2,2-trifluoroethyl
 - 2-methyl-2-propenoate and 3-[3,3,3-trimethyl-1,1-
 - bis[(trimethylsily1)oxy]disiloxany1]propyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)
 - CM 1
 - CRN 163674-37-1
 - CMF C13 H24 N 09 P

CM 2

CRN 17096-07-0

CMF C16 H38 O5 Si4

```
CM 3
   CRN 352-87-4
   CMF C6 H7 F3 O2
F3C_CH2_O_U_U_U_Ma
   CM 4
   CRN 109-16-0
   CMF C14 H22 O6
CM 5
   CRN 97-90-5
   CMF C10 H14 O4
   CM 6
   CRN 80-62-6
   CMF C5 H8 O2
H2C 0
  ICM G02C007-04
   ICS C08F265-06
   63-7 (Pharmaceuticals)
   Section cross-reference(s): 38
  163674-32-6P 163674-34-8P 163674-36-0P 163674-38-2P 163674-40-6P 163716-64-1P 163716-65-2P
   RL: DEV (Device component use); SPN (Synthetic preparation); THU
   (Therapeutic use); BIOL (Biological study); PREP (Preparation);
   USES (Uses)
      (surface coating of contact lenses)
```

L50 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1993:4011 HCAPLUS Full-text DOCUMENT NUMBER: 118:4011

10/596.747-301496-EIC SEARCH ORIGINAL REFERENCE NO.: 118:851a.854a TITLE . Degree of C4 photosynthesis in C4 and C3-C4 Flaveria species and their hybrids. II. Inhibition of apparent photosynthesis by a phosphoenolpyruvate carboxylase inhibitor AUTHOR(S): Brown, R. Harold; Byrd, George T.; Black, Clanton C. CORPORATE SOURCE: Dep. Agron., Univ. Georgia, Athens, GA, 30602, IISA SOURCE: Plant Physiology (1992), 100(2), 947-50 CODEN: PLPHAY: ISSN: 0032-0889 DOCUMENT TYPE: Journal LANGUAGE: English ED Entered STN: 10 Jan 1993 AB Hybrids have been made between species of Flaveria exhibiting varying levels of C4 photosynthesis. The degree of C4 photosynthesis expressed in 4 interspecific hybrids (Flaveria trinervia [C4] + F. linearis [C3-C4], F. brownii [C4-like] + F. linearis, and two three-species hybrids from F. trinervia + [F. brownii + F. linearis]) was estimated by inhibiting phosphoenolpyruvate carboxylase in vivo with 3,3-dichloro-2dihydroxyphosphinoylmethyl-2-propenoate (DCDP). The inhibitor was fed to detached leaves at a concentration of 4 mM, and apparent photosynthesis was measured at atmospheric levels of CO2 and at 20 and 210 mL L-1 of O2. Photosynthesis at 210 mL L-1 of O2 was inhibited 32% by DCDP in F. linearis, by 60% in F. brownii, and by 87% in F. trinervia. Inhibition in the hybrids ranged from 38 to 52%. The inhibition of photosynthesis by 210 mL L-1 of 02 was increased when DCDP was used, except in the C4 species, F. trinervia, in which photosynthesis was insensitive to 02. Except for F. trinervia, control plants with less O2 sensitivity (more C4-like) exhibited a progressively greater change in O2 inhibition of photosynthesis when treated with DCDP. This increased O2 inhibition probably resulted from decreased CO2 concns. in bundle sheath cells due to inhibition of phosphoenolpyruvate carboxylase. The inhibition of photosynthesis by DCDP is concluded to underestimate the degree of C4 photosynthesis in the interspecific hybrids because increased direct assimilation of atmospheric CO2 by ribulose bisphosphate carboxylase may compensate for inhibition of phosphoenolpyruvate carboxylase. 108793-81-3 RL: BIOL (Biological study) (C4 photosynthesis inhibition by, in Flaveria C4 and C3-C4 hybrids) 108793-81-3 HCAPLUS CM 2-Propenoic acid, 3,3-dichloro-2-[(phosphonooxy)methyl]- (CA INDEX NAME) CC12 HO2C_U_CH2_OPO3H2 CC 11-6 (Plant Biochemistry) 108793-81-3 RL: BIOL (Biological study) (C4 photosynthesis inhibition by, in Flaveria C4 and C3-C4 hybrids) L50 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN 1987:419847 HCAPLUS Full-text ACCESSION NUMBER: DOCUMENT NUMBER: 107:19847

ONCIGINAL REFERENCE NO.: 107:32914, 3294

TITLE: 107:32914, 3294

TITLE: propensate, a new, specific inhibitor of phosphoenolpyruvate carboxylase denkins, Colin L. D.; Harris, Roger L. N.; McFadden, Helen G.

CORPORATE SOURCE: Div. Plant Ind., CSTRO, Canberra, 2601,

```
Australia
SOURCE .
                         Biochemistry International (1987).
                         14(2), 219-26
                         CODEN: BIINDF; ISSN: 0158-5231
DOCUMENT TYPE:
                         Journal
LANGUAGE .
                         English
ED Entered STN: 25 Jul 1987
AB
    3,3-Dichloro-2-dihydroxyphosphinoylmethyl-2-propenoate (I) is a potent linear
     competitive inhibitor of maize leaf phosphoenolpyruvate carboxylase [Ki(Mn2+) = 3 μM;
     \text{Ki}\left(\text{Mg2+}\right) = 80 \mu\text{M}]. In contrast, the compound showed no inhibition of pyruvate kinase,
     pyruvate, inorg. phosphate dikinase, phosphoenolpyruvate carboxykinase, or enolase, but
     was an effective inhibitor of phosphoenolpyruvate carboxylase from several C4 and C3
     plant species. Of a range of phosphoenolpyruvate analogs reported as inhibitors, I is
     the only one which shows high selectivity towards phosphoenolpyruvate carboxylase among
     phosphoenolpyruvate-dependent enzymes.
тт
     108793-81-3P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and phosphoenolpyruvate carboxylase inhibition by)
     108793-81-3 HCAPLUS
     2-Propenoic acid, 3,3-dichloro-2-[(phosphonooxy)methyl]- (CA
     INDEX NAME)
 HO2C_U_CH2_OPO3H2
    7-3 (Enzymes)
    108793-81-39
     RL: SPN (Synthetic preparation): PREP (Preparation)
        (preparation and phosphoenolpyruvate carboxylase inhibition by)
L50 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:
                         1986:403039 HCAPLUS Full-text
DOCUMENT NUMBER:
                         105:3039
ORIGINAL REFERENCE NO.: 105:591a,594a
TITLE:
                         Polymerizable phospholipids and their
                         polymeric liposomes
AUTHOR(S):
                         Takane, Minoru; Shigehara, Kiyotaka; Tsuchida,
CORPORATE SOURCE:
                         Dep. Polym. Chem., Waseda Univ., Tokyo, 160,
                         Japan
SOURCE:
                         Makromolekulare Chemie (1986),
                         187(4), 853-62
                         CODEN: MACEAK: ISSN: 0025-116X
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
     Entered STN: 13 Jul 1986
AB
     Phospholipids containing polymerizable itaconate moieties were synthesized and their
     formation of liposomes was studied. Although the itaconate phospholipids alone form
     rather unstable liposomes by ultrasonication, mixts, with other phospholipids such as
     dipalmitoyl phosphatidylcholine, bis(2,4-octadienoyl) phosphatidylcholine or
     cholesterol, form stable and single-wall, small sized liposomes. The polymerizability
     of itaconate phospholipids and the stabilization of such mixed liposomes are discussed.
   102610-88-8P
    RL: PREP (Preparation)
        (preparation of, for liposomes)
     102610-88-8 HCAPLUS
CM
     3, 5, 8, 12-Tetraoxa-4-phosphahexacosan-1-aminium,
     4-hvdroxv-N, N, N-trimethvl-10-methvlene-9, 11-dioxo-6-[[(1-
     oxooctadecvl)oxvlmethvl]-, inner salt, 4-oxide, homopolymer (9CI)
     (CA INDEX NAME)
    CM
```

CRN 102610-87-7 CMF C44 H84 N O10 P

9-10 (Biochemical Methods)

Section cross-reference(s): 23, 27

102583-28-8P 102583-30-2P 102583-32-4P 102610-88-8P RL: PREP (Preparation)

(preparation of, for liposomes)

L50 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1980:176403 HCAPLUS Full-text

DOCUMENT NUMBER: 92:176403

ORIGINAL REFERENCE NO.: 92:28519a,28522a TITLE .

The peroxidatic reaction catalyzed by horse liver alcohol dehydrogenase. 3. Nuclear

magnetic resonance spectroscopic study of NADX AUTHOR(S): Mazzini, Alberto; Dradi, Emanuele; Favilla,

Roberto: Fava, Adriano: Cavatorta, Paolo:

Abdallah, Mohamed A.

CORPORATE SOURCE:

Unita Biofis. Mol., Univ. Parma, Parma,

I-43100, Italy SOURCE . European Journal of Biochemistry (1980

), 104(1), 229-35

CODEN: EJBCAI: ISSN: 0014-2956

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984 GT

As previously reported, horse liver alc. dehydrogenase catalyzes a reaction between NAD and H202. The final isolated product is called NADX because of its unknown structure. The results of spectroscopic investigations on this compound are described. They indicated that only the nicotinamide moiety of the original NAD mol. was modified by the action of H202. From the 1H and 13C NMR spectra of NADX, the structure I was deduced. This structure was consistent with both UV and reactivity measurements performed on NADX. A tentative mechanism for the whole peroxidatic reaction pathway leading to NADX was proposed. TT 73435-45-7

RL: BIOL (Biological study)

(enzymic formation and structure of)

RN 73435-45-7 HCAPLUS

CN Adenosine 5'-(trihydrogen diphosphate), P'→5'-ester with 2-formyl-3-(β-D-ribofuranosylamino)-2-propenamide (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-B

__ NH 2

CC 7-3 (Enzymes)

IT 73435-45-7 RL: BIOL (Biological study)

(enzymic formation and structure of)

FULL SEARCH HISTORY

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=> d his nofile
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L21

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                D SCA
                SEL RN
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                6/BI OR 107-21-1/BI OR 112-47-0/BI OR 17435-77-7/BI OR
                752234-97-2/BI OR 752234-98-3/BI OR 752234-99-4/BI OR
                752235-00-0/BI OR 855894-56-3/BI OR 855894-57-4/BI OR
                855894-58-5/BI)
                D SCA
1.3
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                D SCA
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                D RN
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                STR L8
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              0 SEA SSS SAM L5 AND L10
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            50 SEA SSS SAM L5
L13
            36 SEA SSS SAM L8
T.1.4
            50 SEA SSS SAM L5
1.15
         257255 SEA SSS FUL L5
L16
              5 SEA SPE-ON ABB-ON PLU-ON L2 AND L15
              O SEA SUB=L15 SSS SAM L8 AND L5
L18
              0 SEA SUB=L15 SSS SAM L8
                D OUE STAT
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L19
               STR L8
    FILE 'REGISTRY' ENTERED AT 10:56:54 ON 13 JUL 2009
L20
             1 SEA SUB-L15 SSS SAM L19
               D SCA
```

1 SEA SUB=L15 SSS SAM L5 AND L19

```
D SCA
T.22
            30 SEA SUB-L15 SSS FUL L5 AND L19
                D SCA
L23
             0 SEA SUB=L15 SSS SAM L5 AND L8
L24
             18 SEA SUB=L15 SSS FUL L5 AND L8
               SAV TEMP L22 SAS747REG/A
               SAV TEMP L24 SAS747REGA/A
               OUE SPE-ON ABB-ON PLU-ON CH20 OR C2H40 OR C3H60 OR
               C4C80
              6 SEA SPE=ON ABB=ON PLU=ON L24 AND L25
L26
               D SCA
               E OXIRANE/CN
L27
             1 SEA SPE=ON ABB=ON PLU=ON OXIRANE/CN
               D
L28
             2 SEA SPE=ON ABB=ON PLU=ON L24 AND 75-21-8/CRN
               D SCA
                E METHYLOXIRANE/CN
L29
             1 SEA SPE=ON ABB=ON PLU=ON METHYLOXIRANE/CN
               D SCA
T.30
             O SEA SPE=ON ABB=ON PLU=ON L24 AND 75-56-9/CRN
T.31
             2 SEA SPE=ON ABB=ON PLU=ON L22 AND 75-21-8/CRN
             O SEA SPE=ON ABB=ON PLU=ON L22 AND 75-56-9/CRN
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               D SCA L31
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L34
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L36
             22 SEA SPE=ON ABB=ON PLU=ON L35 AND 1/NC
L37
             1 SEA SPE=ON ABB=ON PLU=ON L36 AND C20 H30 O4/MF
               D SCA
               D RSD
               E 553.3/RID
L38
         21108 SEA SPE=ON ABB=ON PLU=ON 553.3/RID
L39
              2 SEA SPE=ON ABB=ON PLU=ON L24 AND L38
               D SCA
               D SCA L24
T.40
              8 SEA SPE=ON ABB=ON PLU=ON L26 OR L28 OR (L30 OR L31
               OR L32) OR L39
               D SCA
L41
            10 SEA SPE=ON ABB=ON PLU=ON L24 NOT L40
               D SCA
L42
             12 SEA SPE=ON ABB=ON PLU=ON L22 NOT L24
                D SCA
            30 SEA SPE=ON ABB=ON PLU=ON L22 OR L24
L43
     FILE 'HCAPLUS' ENTERED AT 11:30:06 ON 13 JUL 2009
L44
               OUE SPE=ON ABB=ON PLU=ON PY=<2003 NOT P/DT
                OUE SPE=ON ABB=ON PLU=ON (PY=<2003 OR PRY=<2003 OR
L45
               AY=<2003 OR MY=<2003 OR REVIEW/DT) AND P/DT
L46
             17 SEA SPE=ON ABB=ON PLU=ON L43
L47
             12 SEA SPE=ON ABB=ON PLU=ON L46 AND (L44 OR L45)
                SAV TEMP L47 SAS747HCP/A
               D OUE STAT L47
L48
             3 SEA SPE-ON ABB-ON PLU-ON L40
             1 SEA SPE=ON ABB=ON PLU=ON L48 AND L47
               D SCA
L50
             12 SEA SPE-ON ABB-ON PLU-ON L49 OR L47
               SAV TEMP L50 SAS747HCP/A
               D QUE STAT L50
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D L50 1-12 IBIB ED ABS HITSTR HITIND